OMBRO README FILE

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Overview

This document provides a brief description of the OMBRO data product. OMBRO contains total column BrO and ancillary information retrieved from OMI global and spatial zoom mode measurements using a retrieval algorithm that is based on non-linear least-squares fitting originally developed for GOME, and adapted for the OMI instrument. In global mode each file contains a single orbit of data covering a swath of approximately 2,600 km wide from pole to pole (sunlit portions only).

Fitting uncertainties for the BrO slant columns typically range between 25-100%, with as low as 5% over BrO hotspots. This is roughly 2-4 times what was achieved from GOME. Uncertainties in the stratospheric air mass factor (AMF), used to convert slant to vertical columns, are estimated to be 10% or less. Hence the total uncertainties of the BrO vertical columns typically range within 27-101%.

Release History and Release-Specific Information

Software Version	1.0.0
ECS Collection Number	2
Public Release	1 February 2007
Validation Release	25 December 2005
Known Issue List	◇ Across-track striping in the data product (see OMSAO_DeStriping_README). ◇ Some correlation with scene albedo Please consult OMSAO_KnownIssues_README for up-to-date information.

Algorithm Description

The algorithm is based on the direct fitting of radiances and irradiances. In particular, and differing from what is commonly referred to as Differential Optical Absorption Spectroscopy (DOAS) fitting, radiances are not divided by irradiances, no logarithms are taken of the spectra, and no high-pass filtering is applied. The three main stages of the algorithm are (1) Solar wavelength calibration, in which the optimum wavelength registration of the solar irradiance measurements is determined and, unless pre-measured laboratory slit function profiles are used (which is the default), the instrument slit function is determined by fitting an asymmetric Gaussian; (2) Radiance wavelength calibration, which finds the optimum wavelength registration for a representative swath of radiance measurements (usually in the middle of the orbit) and determines a common wavelength grid for auxiliary data bases (molecular reference cross sections, *etc*.); and (3) Fitting of all swath lines in the OMI granule. In each stage, the calibration/fitting is performed individually for the 60 cross-track pixels[1] of an OMI swath line. For improved numerical stability, radiances and irradiances are divided by their respective averages over the fitting window; in other words, they are "normalized" to values ~1.

BrO fitting is performed in the spectral window 338-357 nm, within the UV-2 channel of the OMI instrument. The model that is fitted to the measurements consists of the solar irradiance, attenuated by contributions from BrO (the target gas), inelastic (rotational Raman, or *Ring*) scattering, and interferences from other atmospheric gases, including ozone and NO_2; it also contains additive and multiplicative closure polynomials and parameters for spectral shift and squeeze, as well as a sampling correction [Chance *et al*., 2005] that is computed on-line. The fit is mostly unconstrained, with the exception of selected parameters, including the spectral shift, which are constrained in order to prevent problems arising from out-of-bounds values.

1 Alternatively: 30 cross-track pixels in rebinned spatial zoom mode, occurring one day per month.

The results from the spectral fitting are BrO slant columns. These are converted to vertical columns using a look-up table of stratospheric air mass factors (AMFs) that have been pre-computed using climatological BrO profiles. The AMFs used for the conversion are provided in the data product.

The algorithm employs several methods to reduce cross-track striping of the BrO columns. These include outlier screening in the fitting residuals the use of a composite solar spectrum (both employed during the fitting process), as well as a post-processing smoothing of the fitted columns. Particularly the latter method almost certainly introduces an as yet unquantified bias to the fitted columns that the user of the data should be aware of. The smoothed columns are provided in a separate data field, *ColumnAmountDestriped*. For details on all destriping procedures please consult the separate OMSAO_DeStriping_README file.

More details on algorithm specifics can be found in the OMI Algorithm Theoretical Basis Document Vol. 4, and in Kurosu *et al*. [2004].

Data Quality Assessment

Across-track striping (systematically elevated or reduced column values at the same cross track position along the whole track) of the BrO columns is a presently outstanding issue. This is not unique to BrO but affects all OMI data products to a higher or lesser degree. Small absorbers like BrO, HCHO and OClO however, are more strongly affected by striping since the column values are of a similar order of magnitude as the stripes, so that the effect is relatively stronger. Various efforts, both at Level 0-1 and 1-2 data processing, are under way to improve this situation, including the method of outlier identification in the fitting residual as employed in the BrO fit. A satisfactory solution remains still to be found, and users of the BrO columns provided here must be aware of this issue.

The BrO data product provides RMS and one standard deviation (1σ) fitting uncertainties, as derived from the fitting covariance matrix. These uncertainties do not include contributions from uncertainties in the measurements or the reference cross sections. In addition to the uncertainties, a fitting diagnostic flag (*FitConvergenceFlag*) provides information on (non-)convergence of the fitting process. This flag should be consulted for more details on the quality of a particular BrO column datum. For details see the product specification document OMBRO.fs or consult the File Specification README.

Preliminary Validation

Several validation activities for the OMI BrO product are ongoing. These include comparisons with other satellite instruments (GOME and SCIAMACHY) as well as comparisons with ground-based measurements. At present, only preliminary results from satellite comparisons are available.

Direct comparisons with GOME data products are difficult since BrO retrievals from GOME are no longer reliable due to the advanced degradation of the GOME instrument. However, vertical columns of ~$2\text{-}4 \bullet 10^{13}$ mol/cm^2 retrieved from OMI around the equator (where global BrO distributions are at a minimum) and ~$1.5\text{-}2 \bullet 10^{14}$ mol/cm^2 in isolated hot-spots like shelf-ice areas in polar regions during polar Spring, are in agreement with what has been observed from GOME in the past. First comparisons with BrO columns from SCIAMACHY show good agreement for both individual granules and monthly averages.

BrO Sample Images

A number of sample images of daily BrO distributions over the North and South Poles for selected days in 2006 can be found on the OMI BrO Sample Image Page.

Which Data Should Be Used?

All SAO data products (BrO, HCHO, OClO) contain the data field *MainDataQualityFlag* that should aid the user in the selection of which data to use and which to avoid. Each ground pixel is assigned a value, the range and classification of which are as follows:

Value	Classification	Rationale
0	Good	All quality checks passed; data may be used with confidence
1	Suspect	Caution advised because one or more of the following conditions are present: • *FitConvergenceFlag* is < 300 (but > 0): convergence at noise level • Column+1σ uncertainty < 0
2	Bad	Avoid using data because one or more of the following conditions are present: • *FitConvergenceFlag* is < 0: abnormal termination, no convergence • Column+2σ uncertainty < 0
-1	Missing	No column values have been computed; entries are missing

Product Description

A 2600 km wide OMI swath contains 60 cross-track pixels, ranging in size from 14x24 km^2 (along x across track) in the center of the swath to about 28x150 km^2 at the edges of the swath (median: 15x33 km^2). The pixels on the swath are not symmetrically aligned on the line perpendicular to the orbital plane. However, the latitude and longitude provided with each pixel represents the location of each pixel on the ground to a fraction of a pixel.

The OMBRO product is written as HDF-EOS5 swath file. A single OMBRO file contains information retrieved from each OMI pixel over the sun-lit portion of the orbit (a.k.a. an *OMI granule*). The information provided in these files include: Geodetic longitude and latitude, solar and line-of-sight zenith and azimuth angles, total column BrO with RMS and 1σ fitting uncertainties, longitude and latitude corner coordinates for each OMI pixel, and a range of ancillary parameters that provide information to assess data quality. Average values over an OMI granule for the BrO total column, uncertainties, and RMS, as well as the percent values of "good" (converged and columns positive within 2σ fitting uncertainties; this includes the "suspect" category from the table above) and "bad" (failed convergence or truly negative columns) provide general, granule-based information on data quality. For a complete list of data fields and their description, please read the file specifications OMBRO.fs or see the File Specification README.

OMBRO data are publicly available from NASA's OMI/Aura Data Products Web Page (GES-DISC). Also, subsets of these data over many ground stations and along Aura validation aircraft flight paths are available through the Aura Validation Data Center (AVDC) website to those investigators who are associated with the various Aura science teams.

For questions and comments related to the OMBRO dataset please contact Thomas P. Kurosu. Please send a copy of your e-mail to Kelly Chance, who has the overall responsibility for this product.

References

OMI Algorithm Theoretical Basis Document, Volume IV, OMI Trace Gas Algorithms, OMI-ATBD-VOL4, ATBD-OMI-04, Version 2.0, August 2002.

K. Chance, T.P. Kurosu, and C.E. Sioris, Undersampling correction for array-detector based satellite spectrometers, Applied Optics 44(7), 1296-1304 (2005).

T.P. Kurosu, K. Chance, and C.E. Sioris, "Preliminary results for HCHO and BrO from the EOS-Aura Ozone Monitoring Instrument", in *Passive Optical Remote Sensing of the Atmosphere and Clouds IV, Proc. of SPIE Vol. 5652* (2004), doi: 10.1117/12.578606.